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LOGIN: [redacted]

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	MAY 01	New CAS web site launched
NEWS 3	MAY 08	CA/CAplus Indian patent publication number format defined
NEWS 4	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 5	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS 6	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS 7	MAY 21	CA/CAplus enhanced with additional kind codes for German patents
NEWS 8	MAY 22	CA/CAplus enhanced with IPC reclassification in Japanese patents
NEWS 9	JUN 27	CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 10	JUN 29	STN Viewer now available
NEWS 11	JUN 29	STN Express, Version 8.2, now available
NEWS 12	JUL 02	LEMBASE coverage updated
NEWS 13	JUL 02	LMEDLINE coverage updated
NEWS 14	JUL 02	SCISEARCH enhanced with complete author names
NEWS 15	JUL 02	CHEMCATS accession numbers revised
NEWS 16	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS 17	JUL 16	CAplus enhanced with French and German abstracts
NEWS 18	JUL 18	CA/CAplus patent coverage enhanced
NEWS 19	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 20	JUL 30	USGENE now available on STN
NEWS 21	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 22	AUG 06	BEILSTEIN updated with new compounds
NEWS 23	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 24	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 25	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 26	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 27	AUG 27	USPATOLD now available on STN
NEWS 28	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 29	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index

NEWS EXPRESS 05 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 05 SEPTEMBER 2007.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:54:49 ON 10 SEP 2007

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:55:16 ON 10 SEP 2007
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 SEP 2007 HIGHEST RN 946489-93-6
DICTIONARY FILE UPDATES: 9 SEP 2007 HIGHEST RN 946489-93-6

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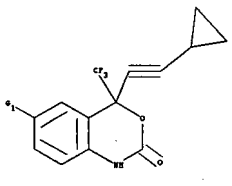
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

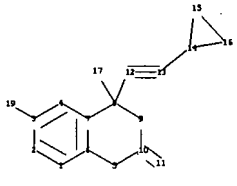
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10732767.str





chain nodes :
11 12 13 17 19
ring nodes :
1 2 3 4 5 6 7 8 9 10 14 15 16
chain bonds :
3-19 8-12 8-17 10-11 12-13 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-6 5-10 6-7 7-8 8-9 9-10 14-15 14-16 15-16
exact/norm bonds :
3-19 5-6 5-10 7-8 8-9 9-10 10-11 14-15 14-16 15-16
exact bonds :
8-12 8-17 12-13 13-14
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
containing 1 :

G1:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:CLASS 19:CLASS

L1 STRUCTURE UPLOADED

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=> d l1
L1 HAS NO ANSWERS
L1                STR
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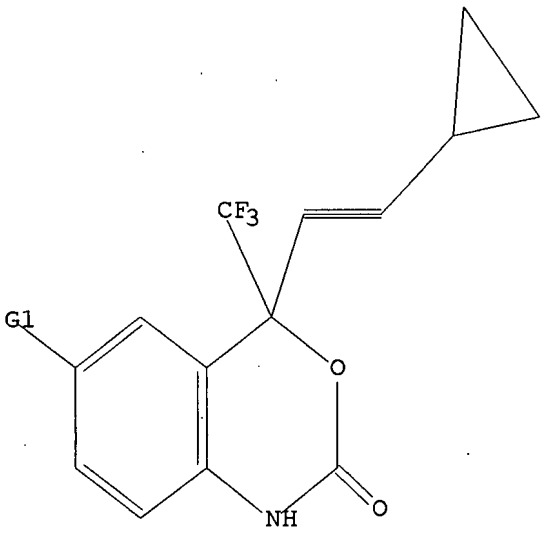


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G1 O,N

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 17:55:35 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        1 TO ITERATE

100.0% PROCESSED         1 ITERATIONS                                 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            1 TO       80
PROJECTED ANSWERS:               1 TO       80

L2             1 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 17:55:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       44 TO ITERATE

100.0% PROCESSED        44 ITERATIONS                                21 ANSWERS
SEARCH TIME: 00.00.01

L3            21 SEA SSS FUL L1

=> FIL CAPLUS
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   172.10     172.31

FILE 'CAPLUS' ENTERED AT 17:55:51 ON 10 SEP 2007
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FILE COVERS 1907 - 10 Sep 2007 VOL 147 ISS 12
FILE LAST UPDATED: 9 Sep 2007 (20070909/ED)

=> s l3
L4 11 L3

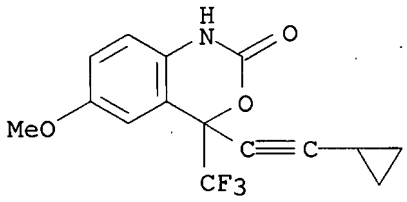
=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:739365 CAPLUS
DOCUMENT NUMBER: 145:347790
TITLE: QSAR for non-nucleoside inhibitors of HIV-1 reverse transcriptase
AUTHOR(S): Duchowicz, Pablo R.; Fernandez, Michael; Caballero, Julio; Castro, Eduardo A.; Fernandez, Francisco M.
CORPORATE SOURCE: INIFTA, Division Quimica Teorica, Departamento de Quimica, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, La Plata, 1900, Argent.
SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(17), 5876-5889
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB By QSAR algorithms we model the potency pIC90 [mM] of 154 non-nucleoside reverse transcriptase inhibitors (NNRTI) of the wild-type HIV-1 virus, considered as the second generation analogs of Efavirenz. In addition, 56 inhibitors of the K-103N viral mutant form are also investigated. A pool of 1494 theor. mol. descriptors provided mainly by the Dragon 5 software is explored by several methods of variable selection: forward stepwise regression, the replacement method, and the genetic algorithm approach. The optimal models found include up to seven parameters: R = 0.7991, R1-20%-o = 0.7233 for the case of wild-type, and R = 0.9261, R1-5%-o = 0.8802 for the K-103N mutation.

IT 205754-67-2 205754-76-3 205754-95-6
256417-70-6 256417-74-0 256417-78-4
256417-80-8
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR for non-nucleoside inhibitors of HIV-1 reverse transcriptase)

RN 205754-67-2 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-methoxy-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 205754-76-3 CAPLUS
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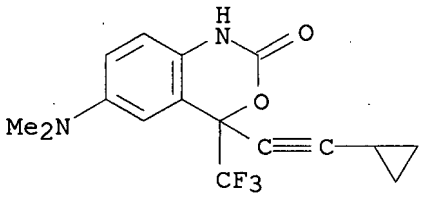

RN 205754-95-6 CAPLUS
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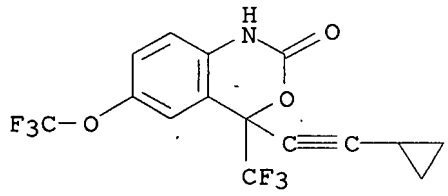

RN 256417-70-6 CAPLUS
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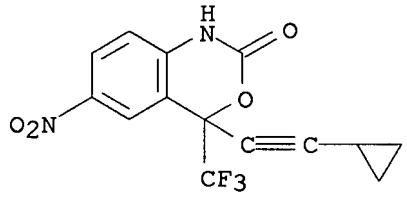

RN 256417-74-0 CAPLUS
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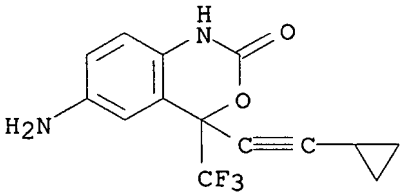
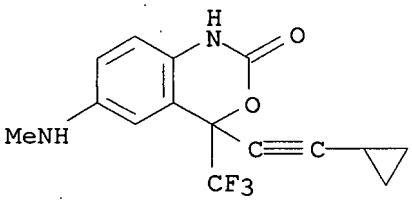
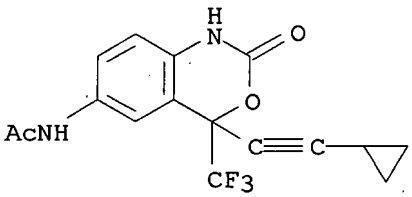


RN 256417-78-4 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-(methylamino)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 256417-80-8 CAPLUS
CN Acetamide, N-[4-(cyclopropylethynyl)-1,4-dihydro-2-oxo-4-(trifluoromethyl)-2H-3,1-benzoxazin-6-yl]- (9CI) (CA INDEX NAME)



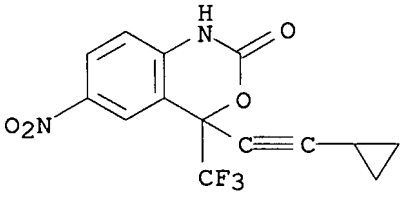
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:398843 CAPLUS
DOCUMENT NUMBER: 145:330429
TITLE: A QSAR study on benzoxazinones, analogues of efavirenz, for the discovery of potent HIV-1 reverse transcriptase inhibitors
AUTHOR(S): Srivastava, A. K.; Khan, Arbab A.; Tripathi, Abha; Chaurasia, Shraddha
CORPORATE SOURCE: QSAR Research Laboratory, Department of Chemistry, University of Allahabad, Allahabad, 211002, India
SOURCE: Journal of Saudi Chemical Society (2006), 9(3), 571-574
CODEN: JSCSFO; ISSN: 1319-6103
PUBLISHER: Saudi Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The anti HIV-1 activity of Benzoxazinones, analogs of Efavirenz, is analyzed in relation to their physicochem. and mol. properties. The activities of the compds. are found to be significantly correlated with steric parameter, mol. connectivity $^1\chi v$, hydrophobicity-log P and electronic parameter equalized electro negativity-Xeq. The results are found to be useful in discussing the mechanism of drug-receptor

interaction.

IT 256417-70-6 256417-74-0 256417-78-4
256417-80-8
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(QSAR study on benzoxazinones, analogs of efavirenz, for discovery of potent HIV-1 reverse transcriptase inhibitors)

RN 256417-70-6 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-nitro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 256417-74-0 CAPLUS
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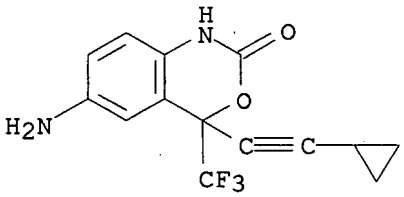
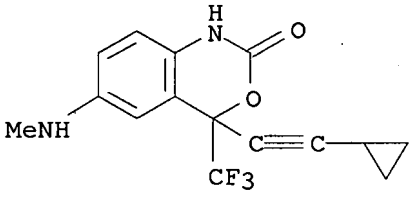
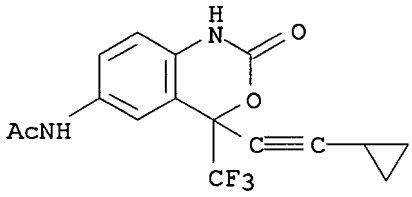


RN 256417-78-4 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-(methylamino)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 256417-80-8 CAPLUS
CN Acetamide, N-[4-(cyclopropylethynyl)-1,4-dihydro-2-oxo-4-(trifluoromethyl)-2H-3,1-benzoxazin-6-yl]- (9CI) (CA INDEX NAME)



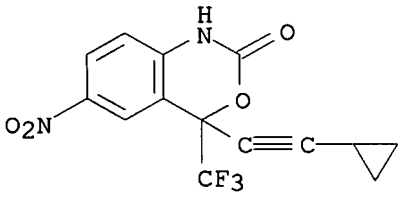
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1179261 CAPLUS
DOCUMENT NUMBER: 144:100351
TITLE: 3D-QSAR studies of benzoxazinones: Analogs of efavirenz
AUTHOR(S): Jacob, Reena Rachel; Kumar, Surendra; Tiwari, Meena
CORPORATE SOURCE: Department of Pharmacy, Shri Govindram Seksaria Institute of Technology and Science, Indore, 452 003, India
SOURCE: Asian Journal of Chemistry (2005), 17(2), 1031-1040
CODEN: AJCHEW; ISSN: 0970-7077
PUBLISHER: Asian Journal of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

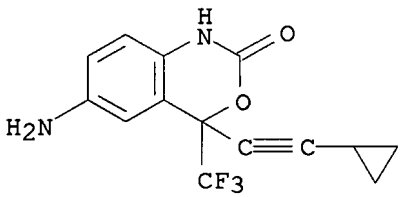
AB In the present study, a set of 14 analogs of Efavirenz with human immunodeficiency virus-1 (HIV-1) reverse transcriptase (RT) inhibitory activity, were subjected to 3D-QSAR studies. Various combinations of thermodn., electronic and steric descriptors were used in order to understand the physicochem. properties desirable for interaction with the receptor. Multiple linear regression anal. was performed, using VALSTAT, to select the descriptors and to generate various models that relate the structural features to the biol. activity. Among them, an informative and statistically significant model both in fitting and predictive ability (r = 0.9354 and rcv2 = 0.8059) was selected. Cross-validation was performed using leave-one-out (LOO) and bootstrapping method. The significant model indicated that the thermodn. descriptors, viz., Henry's law constant and stretch bend energy play an important role in RT inhibitory activity. Consequently, the best QSAR model will be of major importance to aid the design of new HIV-1 reverse transcriptase inhibitor.

IT 256417-70-6 256417-74-0 256417-78-4
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3D-QSAR studies of benzoxazinones, analogs of efavirenz)

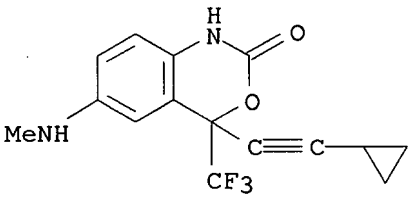
RN 256417-70-6 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-nitro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 256417-74-0 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 6-amino-4-(cyclopropylethynyl)-1,4-dihydro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 256417-78-4 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-(methylamino)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

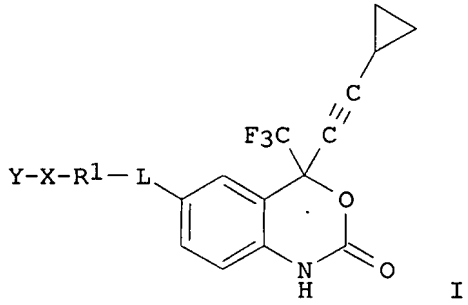


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:527459 CAPLUS
DOCUMENT NUMBER: 143:43890
TITLE: Preparation of 4-cyclopropylethynyl-6-hydroxy-4-trifluoromethyl-1,4-dihydrobenzo[d][1,3]oxazin-2-one derivatives as reagents for detecting efavirenz
INVENTOR(S): Ghoshal, Mitali; Sigler, Gerald; Ouyang, Anlong; Root, Richard
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 19 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005131216	A1	20050616	US 2003-732767	20031210
CA 2489266	A1	20050610	CA 2004-2489266	20041206
EP 1542012	A1	20050615	EP 2004-28897	20041207
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
JP 2005225864	A	20050825	JP 2004-358924	20041210

PRIORITY APPLN. INFO.: US 2003-732767 A 20031210
OTHER SOURCE(S): CASREACT 143:43890; MARPAT 143:43890
GI



I

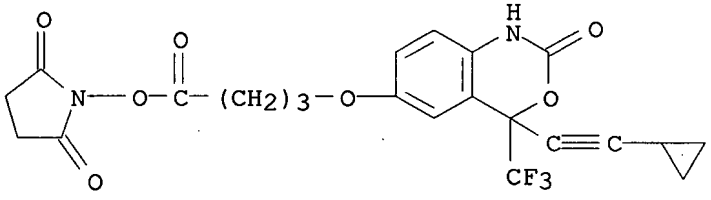
AB The invention provides derivs. of efavirenz (I) [wherein L = NH, O; R1 =

(un)saturated, (un)substituted, straight or branched chain of 0-10 carbon or hetero atoms; X = a linker group consisting of 0-2 substituted or unsubstituted aromatic rings or aliphatic linking groups containing 0-10 carbon or hetero atoms; Y = an activated ester, maleimido group, thiol, or NH-Z (where Z = a carrier or a label)] and methods of making efavirenz derivs. The derivs. I include immunogenic compds. for producing antibodies to efavirenz and labeled efavirenz tracers. These compds. are useful in immunoassay methods for determining efavirenz. Thus, [2-(3-cyclopropyl-1-hydroxy-1-trifluoromethylprop-2-ynyl)-4-(2-methoxyethoxymethoxy)phenyl]carbamic acid tert-Bu ester was cyclized in toluene by treatment with BuLi/hexane at 0-4° for 10 min and at reflux for 1 h to give 4-cyclopropylethynyl-6-(2-methoxyethoxymethoxy)-4-trifluoromethyl-1,4-dihydrobenzo[d][1,3]oxazin-2-one which was deprotected by treatment with CF3CO2H, etherified with Et 4-bromobutyrate in the presence of 18-crown-6 and K2CO3 in acetone at 56° for 3 h, hydrolyzed with LiOH in 50% aqueous MeOH, and acidified with 1 N aqueous HCl to give 4-[(4-cyclopropylethynyl-2-oxo-4-trifluoromethyl-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl)oxy]butyric acid (II). II was esterified with O-(N-succinimidyl)-N,N,N',N'-tetramethyluronium tetrafluoroborate in the presence of diisopropylethylamine in THF to give 4-[[4-(cyclopropylethynyl)-2-oxo-4-trifluoromethyl-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl]oxy]butyric acid 2,5-dioxopyrrolidin-1-yl ester (III). A conjugate prepared from III and keyhole limpet hemocyanin was used to prepare a monoclonal antibody EFA 97.1 specific to efavirenz. The monoclonal antibody EFA 97.1 thus prepared exhibited 100% cross-activity to chiral efavirenz but 0% activity to 3'-azido-3'-deoxythymidine, 2',3'-didehydro-3'-deoxythymidine, nevirapine, delaviridine, nelfinavir, saquinavir, indinavir, ritonavir, amprenavir, lopinavir, and atazanavir which are often coadministered with efavirenz. A serum sample of .apprx.0.2 μL is sufficient to determine efavirenz concentration at 0.0004 to 0.1 μM in a competitive inhibition immunoassay using monoclonal antibody EFA 97.1.

IT 853655-85-3DP, 4-[[4-(Cyclopropylethynyl)-2-oxo-4-trifluoromethyl-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl]oxy]butyric acid 2,5-dioxopyrrolidin-1-yl ester, conjugates with bovine serum albumin
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of efavirenz derivs. as reagents for detecting efavirenz by immunoassay)

RN 853655-85-3 CAPLUS

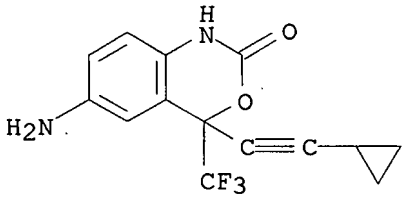
CN 2,5-Pyrrolidinedione, 1-[4-[[4-(cyclopropylethynyl)-1,4-dihydro-2-oxo-4-(trifluoromethyl)-2H-3,1-benzoxazin-6-yl]oxy]-1-oxobutoxy]- (9CI) (CA INDEX NAME)



IT 256417-74-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of efavirenz derivs. as reagents for detecting efavirenz by immunoassay)

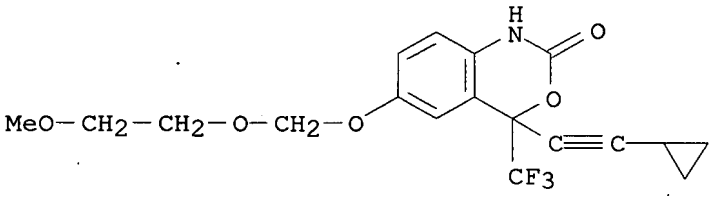
RN 256417-74-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-amino-4-(cyclopropylethynyl)-1,4-dihydro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

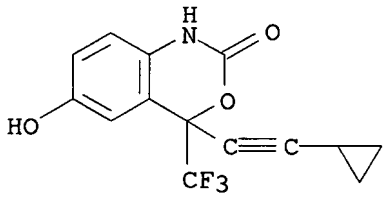


IT 853655-81-9P, 4-Cyclopropylethynyl-6-(2-methoxyethoxymethoxy)-4-trifluoromethyl-1,4-dihydrobenzo[d][1,3]oxazin-2-one 853655-82-0P, 4-Cyclopropylethynyl-6-hydroxy-4-trifluoromethyl-1,4-dihydrobenzo[d][1,3]oxazin-2-one 853655-83-1P, 4-[[4-(Cyclopropylethynyl)-2-oxo-4-trifluoromethyl-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl]oxy]butyric acid ethyl ester 853655-84-2P, 4-[[4-(Cyclopropylethynyl)-2-oxo-4-trifluoromethyl-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl]oxy]butyric acid 853655-85-3P, 4-[[4-(Cyclopropylethynyl)-2-oxo-4-trifluoromethyl-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl]oxy]butyric acid 2,5-dioxopyrrolidin-1-yl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of efavirenz derivs. as reagents for detecting efavirenz by immunoassay)

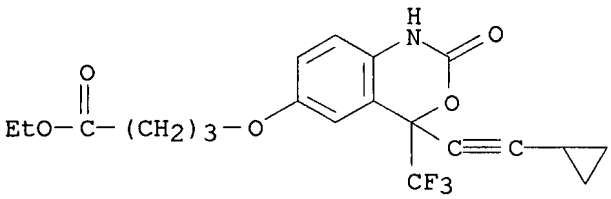
RN 853655-81-9 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-[(2-methoxyethoxy)methoxy]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



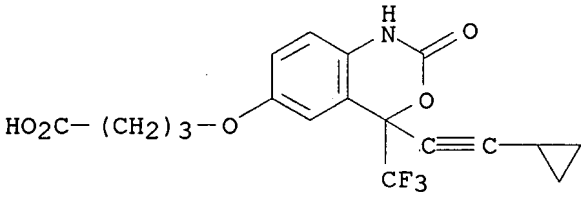
RN 853655-82-0 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-hydroxy-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



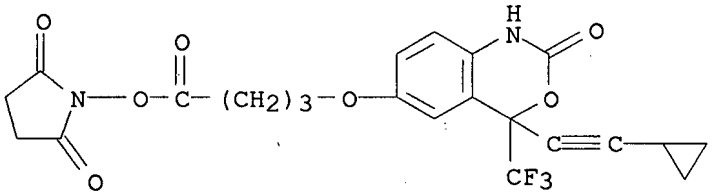
RN 853655-83-1 CAPLUS
CN Butanoic acid, 4-[[4-(cyclopropylethynyl)-1,4-dihydro-2-oxo-4-(trifluoromethyl)-2H-3,1-benzoxazin-6-yl]oxy]-, ethyl ester (9CI) (CA INDEX NAME)



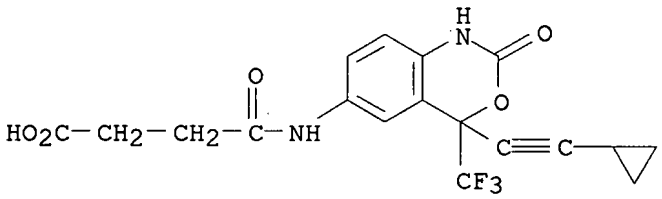
RN 853655-84-2 CAPLUS
CN Butanoic acid, 4-[[4-(cyclopropylethynyl)-1,4-dihydro-2-oxo-4-(trifluoromethyl)-2H-3,1-benzoxazin-6-yl]oxy]- (9CI) (CA INDEX NAME)



RN 853655-85-3 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[4-[[4-(cyclopropylethynyl)-1,4-dihydro-2-oxo-4-(trifluoromethyl)-2H-3,1-benzoxazin-6-yl]oxy]-1-oxobutoxy]- (9CI) (CA INDEX NAME)

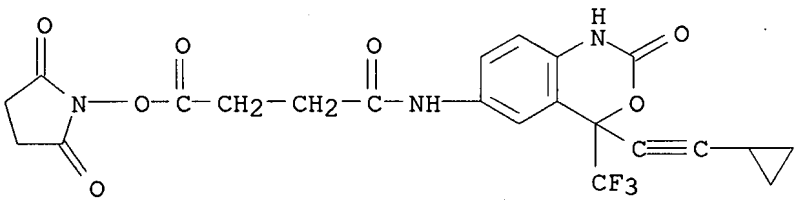


IT 853655-86-4P, N-[4-(Cyclopropylethynyl)-2-oxo-4-trifluoromethyl-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl]succinamic acid 880762-47-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of efavirenz derivs. as reagents for detecting efavirenz by immunoassay)
RN 853655-86-4 CAPLUS
CN Butanoic acid, 4-[[4-(cyclopropylethynyl)-1,4-dihydro-2-oxo-4-(trifluoromethyl)-2H-3,1-benzoxazin-6-yl]amino]-4-oxo- (9CI) (CA INDEX NAME)



RN 880762-47-0 CAPLUS
CN Butanamide, N-[4-(cyclopropylethynyl)-1,4-dihydro-2-oxo-4-(trifluoromethyl)-2H-3,1-benzoxazin-6-yl]-4-[(2,5-dioxo-1-

pyrrolidinyl)oxy]-4-oxo- (9CI) (CA INDEX NAME)



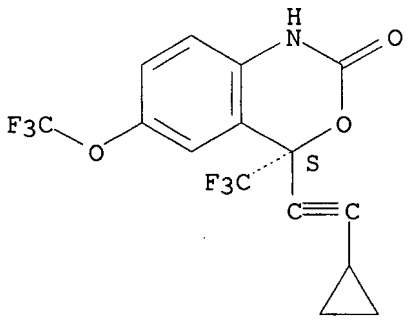
L4 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:387735 CAPLUS
DOCUMENT NUMBER: 143:108975
TITLE: Molecular mechanics PBSA ligand binding energy and interaction of Efavirenz derivatives with HIV-1 reverse transcriptase
AUTHOR(S): Weinzinger, Philipp; Hannongbua, Supa; Wolschann, Peter
CORPORATE SOURCE: Institute for Theoretical Chemistry and Structural Biology, University of Vienna, Vienna, 1090, Austria
SOURCE: Journal of Enzyme Inhibition and Medicinal Chemistry (2005), 20(2), 129-134
CODEN: JEIMAZ; ISSN: 1475-6366
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In order to evaluate the properties of several HIV-1 reverse transcriptase(RT) inhibitors, Efavirenz (SUSTIVA) and a set of its derivs. (benzoxazinones) have been placed into the non-nucleoside analog binding site of the enzyme by mol. docking. The resulting geometries were used for a mol. dynamics simulation and binding energy calcns. The enzyme-inhibitor binding energies were estimated from exptl. inhibitory activities (IC90). The correlation of the predicted and exptl. binding energies were satisfactory acceptable as indicated by r2 = 0.865. Based on MD simulations, the obtained results indicate that the tight association of the ligand to the HIV-1 RT binding pocket was based on hydrogen bonding between Efavirenz's N1 and the oxygen of the backbone of Lys 101, with an estimated average distance of 1.88 Å. Moreover, electrostatic interaction was mainly contributed by two amino acid residues in the binding site; Lys 101 and His 235. MD simulations open the possibility to study the reaction of the flexible enzyme to those substances as well as the overall affinity.

IT 445468-50-8 445468-55-3 445468-61-1
445468-67-7 445468-74-6
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(mol. mechanics PBSA ligand binding energy and interaction of Efavirenz derivs. with HIV-1 reverse transcriptase)

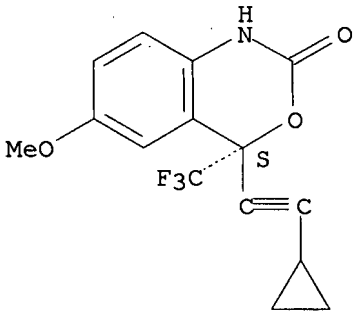
RN 445468-50-8 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-(trifluoromethoxy)-4-(trifluoromethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



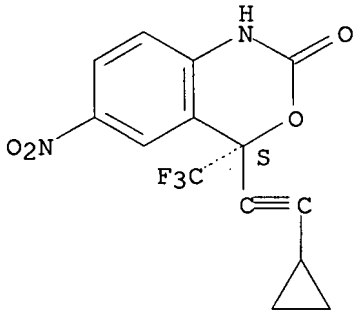
RN 445468-55-3 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-methoxy-4-(trifluoromethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



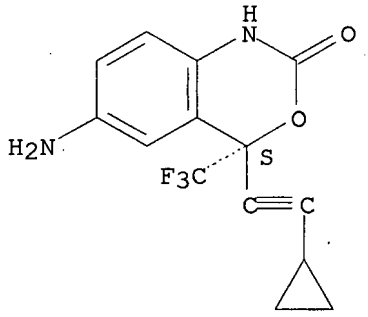
RN 445468-61-1 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-nitro-4-(trifluoromethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



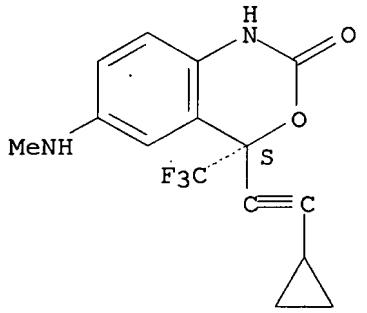
RN 445468-67-7 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 6-amino-4-(cyclopropylethynyl)-1,4-dihydro-4-(trifluoromethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 445468-74-6 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-(methylamino)-4-(trifluoromethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:967787 CAPLUS
DOCUMENT NUMBER: 142:48494
TITLE: QSAR modelling of HIV-1 reverse transcriptase inhibition by benzoxazinones using a combination of P_VSA and pharmacophore feature descriptors
AUTHOR(S): Balaji, S.; Karthikeyan, C.; Hari Narayana Moorthy, N. S.; Trivedi, Piyush
CORPORATE SOURCE: S.G.S.I.T.S., Department of Pharmacy, Indore, Madhya Pradesh, 452003, India
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(24), 6089-6094
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

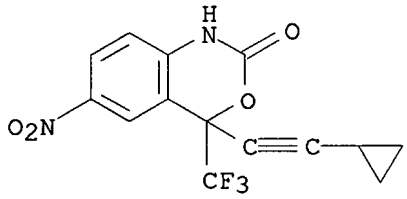
AB In pursuit of better anti-HIV drugs, a quant. structure-activity relationship anal. using a novel set of 2D descriptors was performed on a series of HIV-1 reverse transcriptase inhibitory benzoxazinones. The QSAR models derived from the above mentioned descriptors were found to be statistically significant and exhibited superior predictive power. The results of the study justify the application of the descriptors for exploring the binding mode of the benzoxazinones to the enzyme.

IT 256417-70-6 256417-74-0 256417-78-4
256417-80-8
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(QSAR modeling of HIV-1 reverse transcriptase inhibition by benzoxazinones using van der Waals surface area and pharmacophore feature descriptors)

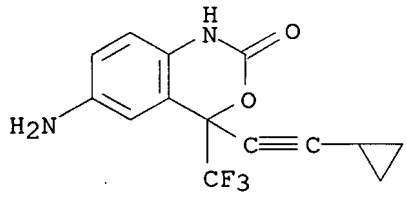
RN 256417-70-6 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-nitro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



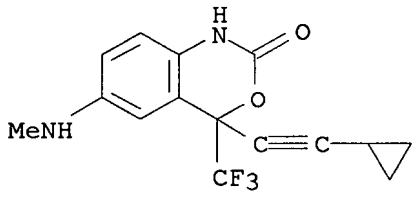
RN 256417-74-0 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-amino-4-(cyclopropylethynyl)-1,4-dihydro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



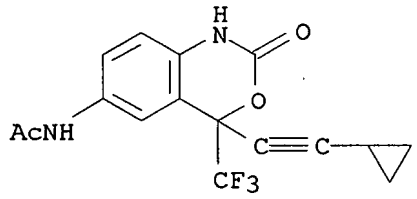
RN 256417-78-4 CAPLUS

CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-(methylamino)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 256417-80-8 CAPLUS

CN Acetamide, N-[4-(cyclopropylethynyl)-1,4-dihydro-2-oxo-4-(trifluoromethyl)-2H-3,1-benzoxazin-6-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

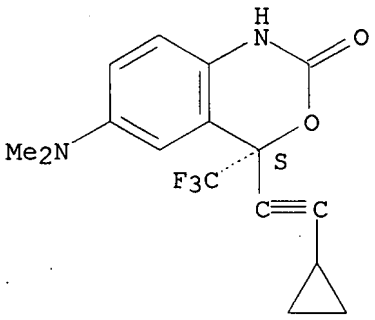
ACCESSION NUMBER: 2002:429780 CAPLUS
DOCUMENT NUMBER: 137:149792
TITLE: Prediction of Activity for Nonnucleoside Inhibitors with HIV-1 Reverse Transcriptase Based on Monte Carlo Simulations
AUTHOR(S): Rizzo, Robert C.; Udier-Blagovic, Marina; Wang, De-Ping; Watkins, Edward K.; Kroeger Smith, Marilyn B.; Smith, Richard H., Jr.; Tirado-Rives, Julian; Jorgensen, William L.
CORPORATE SOURCE: Western Maryland College, Department of Chemistry, and the Department of Chemistry, Yale University, New Haven, CT, 06520-8107, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(14), 2970-2987
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Results of Monte Carlo (MC) simulations for more than 200 nonnucleoside inhibitors of HIV-1 reverse transcriptase (NNRTIs) representing eight diverse chemotypes have been correlated with their anti-HIV activities in an effort to establish simulation protocols and methods that can be used in the development of more effective drugs. Each inhibitor was modeled in a complex with the protein and by itself in water, and potentially useful descriptors of binding affinity were collected during the MC simulations. A viable regression equation was obtained for each data set using an extended linear response approach, which yielded r2 values between 0.54 and 0.85 and an average unsigned error of only 0.50 kcal/mol. The most common descriptors confirm that a good geometrical match between the inhibitor and the protein is important and that the net loss of hydrogen bonds with the inhibitor upon binding is unfavorable. Other phys. reasonable descriptors of binding are needed on a chemotype case-by-case basis. By including descriptors in common from the individual fits, combination regressions that include multiple data sets were also developed. This procedure led to a refined "master" regression for 210 NNRTIs with an r2 of 0.60 and a cross-validated q2 of 0.55. The computed activities show an rms error of 0.86 kcal/mol in comparison with experiment and an average unsigned error of 0.69 kcal/mol. Encouraging results were obtained for the predictions of 27 NNRTIs, representing a new chemotype not included in the development of the regression model. Predictions for this test set using the master regression yielded a q2 value of 0.51 and an average unsigned error of 0.67 kcal/mol. Finally, addnl. regression anal. reveals that use of ligand-only descriptors leads to models with much diminished predictive ability.

IT 445468-49-5 445468-50-8 445468-55-3
445468-61-1 445468-67-7 445468-74-6
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prediction of activity for nonnucleoside inhibitors with HIV-1 reverse transcriptase based on Monte Carlo simulations)

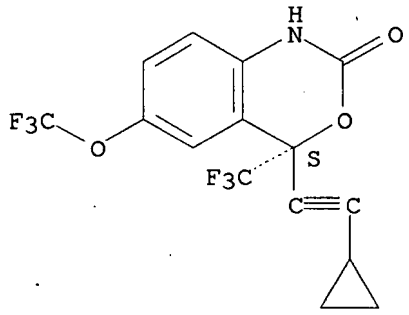
RN 445468-49-5 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-6-(dimethylamino)-1,4-dihydro-4-(trifluoromethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



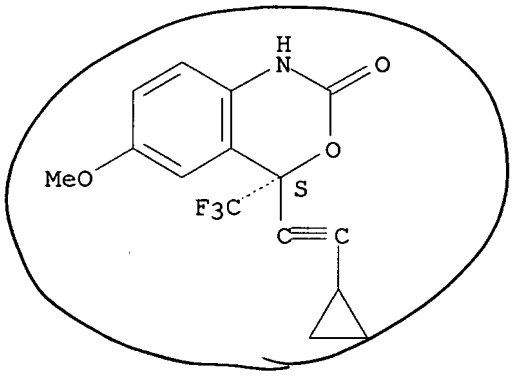
RN 445468-50-8 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-(trifluoromethoxy)-4-(trifluoromethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



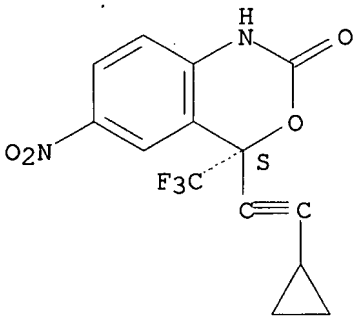
RN 445468-55-3 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-methoxy-4-(trifluoromethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



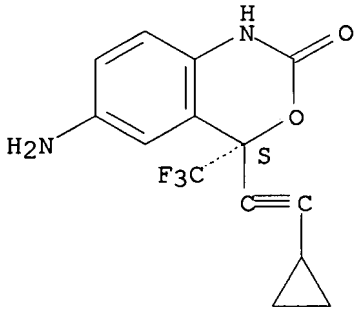
RN 445468-61-1 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-nitro-4-(trifluoromethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



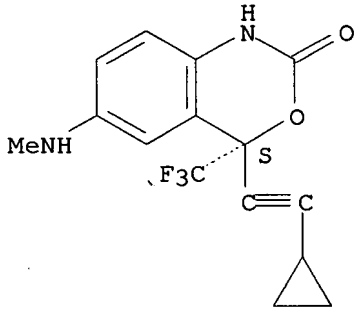
RN 445468-67-7 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 6-amino-4-(cyclopropylethynyl)-1,4-dihydro-4-(trifluoromethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 445468-74-6 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-(methylamino)-4-(trifluoromethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



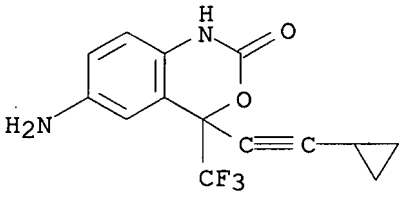
REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:769084 CAPLUS
DOCUMENT NUMBER: 132:117086
TITLE: Synthesis and evaluation of benzoxazinones as HIV-1 reverse transcriptase inhibitors. Analogs of Efavirenz (Sustiva)
AUTHOR(S): Patel, Mona; McHugh, Robert J., Jr.; Cordova, Beverly C.; Klabe, Ronald M.; Erickson-Viitanen, Susan;

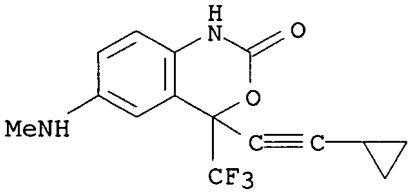
Trainor, George L.; Ko, Soo S.
CORPORATE SOURCE: DuPont Pharmaceuticals Company, Wilmington, DE, 19880-0500, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(22), 3221-3224
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two series of benzoxazinones differing in the aromatic substitution pattern were prepared and evaluated as HIV-1 reverse transcriptase inhibitors and for antiviral activity. The 5-fluoro and 6-nitro substituted compds. displayed activity comparable or better than Efavirenz, the lead structure of the series. Structure-activity relations are discussed.

IT 256417-74-0P 256417-78-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(synthesis and evaluation of benzoxazinones (analogs of Efavirenz (Sustiva)) as HIV-1 reverse transcriptase inhibitors.)

RN 256417-74-0 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 6-amino-4-(cyclopropylethynyl)-1,4-dihydro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

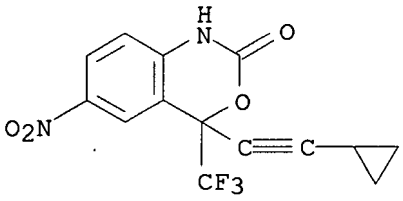


RN 256417-78-4 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-(methylamino)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

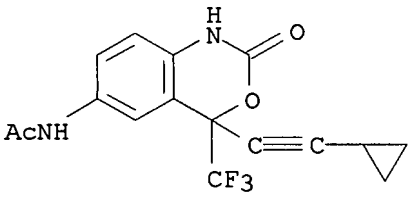


IT 256417-70-6P 256417-80-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and evaluation of benzoxazinones (analogs of Efavirenz (Sustiva)) as HIV-1 reverse transcriptase inhibitors.)

RN 256417-70-6 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-nitro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

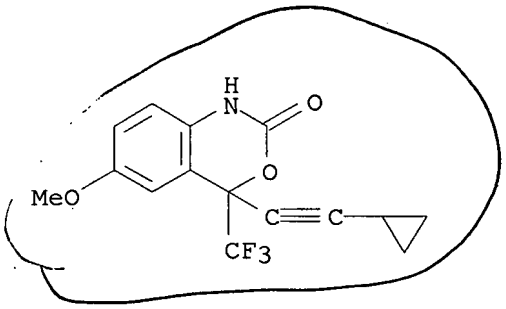


RN 256417-80-8 CAPLUS
CN Acetamide, N-[4-(cyclopropylethynyl)-1,4-dihydro-2-oxo-4-(trifluoromethyl)-2H-3,1-benzoxazin-6-yl]- (9CI) (CA INDEX NAME)

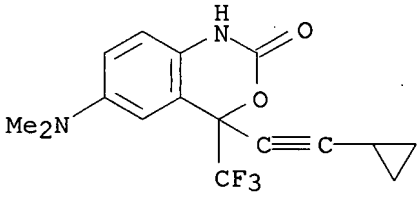


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

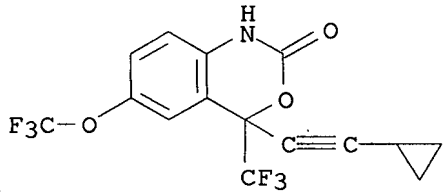
L4 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:662315 CAPLUS
DOCUMENT NUMBER: 132:30313
TITLE: Synthesis and evaluation of analogs of Efavirenz (SUSTIVA) as HIV-1 reverse transcriptase inhibitors
AUTHOR(S): Patel, Mona; Ko, Soo S.; McHugh, Robert J., Jr.; Markwalder, Jay A.; Srivastava, Anurag S.; Cordova, Beverly C.; Klabe, Ronald M.; Erickson-Viitanen, Susan; Trainor, George L.; Seitz, Steven. P.
CORPORATE SOURCE: Experimental Station, DuPont Pharmaceuticals Company, Wilmington, DE, 19880-050, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(19), 2805-2810
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Efavirenz (Sustiva) is a potent non-nucleoside reverse transcriptase inhibitor. Due to the observation of breakthrough mutations of the reverse transcriptase enzyme during Efavirenz therapy, we sought to develop an optimized second generation series. To that end, SAR of the substituents on the aromatic ring was undertaken and the results are summarized here. The 5,6-difluoro and the 6-methoxy substituted benzoxazinones were determined to be equipotent, and as a result such substitution patterns will be incorporated in second generation scaffolds.
IT 205754-67-2P 205754-76-3P 205754-95-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and evaluation of analogs of Efavirenz (Sustiva) as HIV-1 reverse transcriptase inhibitors)
RN 205754-67-2 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-methoxy-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 205754-76-3 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-6-(dimethylamino)-1,4-dihydro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 205754-95-6 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-(trifluoromethoxy)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

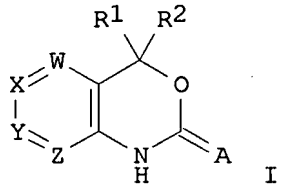
L4 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:136766 CAPLUS
DOCUMENT NUMBER: 130:196659
TITLE: Preparation of 4,4-disubstituted-1,4-dihydro-2H-3,1-benzoxazin-2-ones and related compounds useful as HIV reverse transcriptase inhibitors.
INVENTOR(S): Christ, David Donald; Cocuzza, Anthony Joseph; Ko, Soo Sung; Markwalder, Jay Andrew; Mutlib, Abdul Ezaz; Parsons, Rodney Lawrence, Jr.; Patel, Mona; Seitz, Steven Paul
PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA
SOURCE: U.S., 74 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5874430	A	19990223	US 1997-942031	19971001
US 6140499	A	20001031	US 1998-176491	19981021
US 6303780	B1	20011016	US 2000-627213	20000727

US 2002040138	A1	20020404	US 2001-919065	20010731
US 6492515	B2	20021210		
PRIORITY APPLN. INFO.:			US 1996-27137P	P 19961002
			US 1997-45138P	P 19970430
			US 1997-942031	A3 19971001
			US 1998-176491	A3 19981021
			US 2000-627213	A3 20000727

OTHER SOURCE(S): CASREACT 130:196659; MARPAT 130:196659

GI



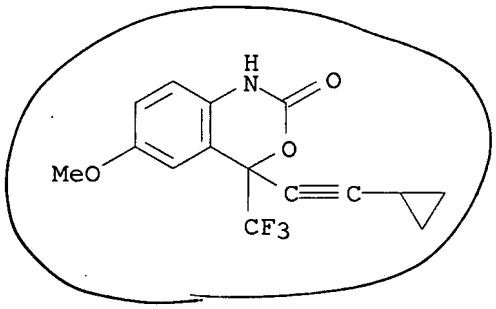
I

AB Title compds. [I; A = O, S; W = N, CR3; X = N, CR4; Y = N, CR5; Z = N, CR6; Q = O, S, NH; R1 = CF3, CF2H, C2F5, alkyl, cycloalkyl, alkenyl, alkynyl; R2 = QCHR7R8, QCHR7C.tplbond.CR8, QCHR7C:CR8, Q(CH2)pCHR7R8, C.tplbond.CR8, CH:CR7R8, (CH2)pCHR7R8, CHR7C.tplbond.CR8, CHR7CH:CHR8, CH:CHCHR7R8; R3 = H, F, Cl, Br, iodo, alkoxy, alkyl; R4 = H, F, Cl, Br, iodo, (substituted) alkyl, alkenyl, alkynyl, alkoxy, OCF3, cyano, NO2, CHO, Ac, COCF3, CONH2, CONHMe, NR7R7a, NR7CO2R7a, CO2R7, SOpR7, SO2NHR7, NR7SO2R7b, Ph, heteroaryl;, R3R4 = OCH2O; R5 = H, F, Cl, Br, iodo; R4R5 = OCH2O, fused benzo ring; R6 = H, OH, alkoxy, cyano, F, Cl, Br, iodo, NO2, CF3, CHO, alkyl, CONH2; R7, R7a = H, alkyl; R8 = H, (substituted) alkyl, CH(OCH2CH2O), alkenyl, cycloalkyl, Ph, heteroaryl; p = 0-2; with provisos], were prepared for treatment of HIV infection (no data). Thus, 5-chloro-1-pentyne in THF at 0° was treated with BuLi; the mixture was warmed to room temperature, cooled to -20°, and treated with 2'-amino-5'-chloro-3'-(tert-butyldimethylsilyloxy)-2,2,2-trifluoroacetophenone (preparation given) in THF followed by 30 min. stirring to give 70% 2-[2-amino-5-chloro-3-(tert-butyldimethylsilyloxy)phenyl]-4-cyclopropyl-1,1,1-trifluoro-3-butyn-2-ol. The latter in PhMe was treated with (Me2CH)2NEt and COCl2 at -25° fo give a residue which was treated with Bu4NF in THF to give 94% 6-chloro-4-(cyclopropylethynyl)-8-hydroxy-4-trifluoromethyl-1,4-dihydro-2H-3,1-benzoxazin-2-one.

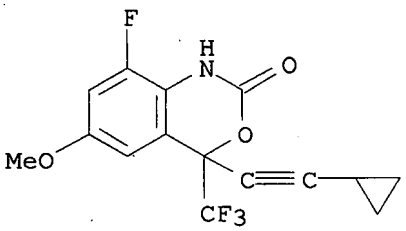
IT 205754-67-2P 205754-75-2P 205754-76-3P
205754-95-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoxazinones and related compds. useful as HIV reverse transcriptase inhibitors)

RN 205754-67-2 CAPLUS

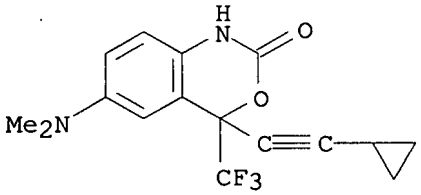
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-methoxy-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



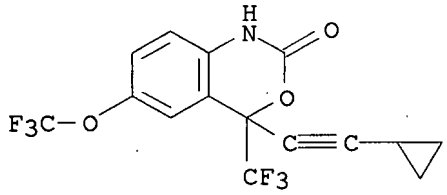
RN 205754-75-2 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-8-fluoro-1,4-dihydro-6-methoxy-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 205754-76-3 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-6-(dimethylamino)-1,4-dihydro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 205754-95-6 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-(trifluoromethoxy)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



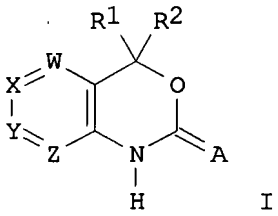
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:219799 CAPLUS
DOCUMENT NUMBER: 128:282840
TITLE: Preparation of 3,1-benzoxazin-2-ones as HIV reverse transcriptase inhibitors
INVENTOR(S): Christ, David Donald; Markwalder, Jay Andrew; Fortunak, Joseph Marian; Ko, Soo Sung; Mutlib, Abdul Ezaz; Parsons, Rodney Lawrence, Jr.; Patel, Mona; Seitz, Steven Paul
PATENT ASSIGNEE(S): Du Pont Merck Pharmaceutical Co., USA
SOURCE: PCT Int. Appl., 213 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9814436	A1	19980409	WO 1997-US17540	19971001
W: AU, BA, CA, CU, JP, LC, MX, NZ				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
ZA 9708759	A	19990330	ZA 1997-8759	19970930
CA 2268953	A1	19980409	CA 1997-2268953	19971001
AU 9748027	A	19980424	AU 1997-48027	19971001
EP 929533	A1	19990721	EP 1997-910726	19971001
EP 929533	B1	20030903		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2001505873	T	20010508	JP 1998-516775	19971001
AT 248826	T	20030915	AT 1997-910726	19971001
EP 1359147	A1	20031105	EP 2003-12262	19971001
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
ES 2203790	T3	20040416	ES 1997-910726	19971001
PRIORITY APPLN. INFO.:			US 1996-725294 A	19961002
			US 1997-846578 A	19970430
			EP 1997-910726 A3	19971001
			WO 1997-US17540 W	19971001

OTHER SOURCE(S): MARPAT 128:282840

GI



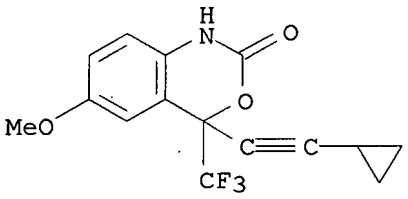
I

AB Title compds. [I; A = O or S; R1 = CF3, (cyclo)alkyl, alkenyl, etc.; R2 = QCHR7R8, QCHR7C.tplbond.R8, CH:CR7R8, etc.; Q = O, S, NH; R7 = H or alkyl; R8 = H, (cyclo)alkyl, Ph, heteroaryl, etc.; W = N or CR3; R3 = H, halo, alkyl, alkoxy; X = N or CR4; R4 = H, halo, alkyl, alkoxy, etc.; Y = N or CR5; R5 = H or halo; R4R5 = OCH2O or CH:CHCH:CH; Z = N or CR6 = H, halo, OH, alkoxy, etc.; ≤2 of W-Z = N] were prepared as HIV reverse transcriptase inhibitors (no data). Thus, 4,3-Cl(MeO)C6H3NHCOCMe3 (preparation given) was C-acylated by CF3CO2Et and the product converted in 3 steps to 3,5-Cl(Me3CMe2SiO)C6H3COCF3 which was treated with BuLi/HC.tplbond.C(CH2)3Cl and the product cyclocondensed with COCl2 to give I [A = O, R1 = CF3, R2 = cyclopropylethynyl, W = Y = CH, X =CCl, Z = C(OH)].

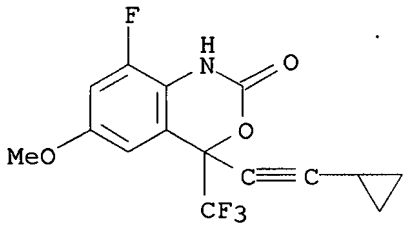
IT 205754-67-2P 205754-75-2P 205754-76-3P
205754-95-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3,1-benzoxazin-2-ones as HIV reverse transcriptase inhibitors)

RN 205754-67-2 CAPLUS

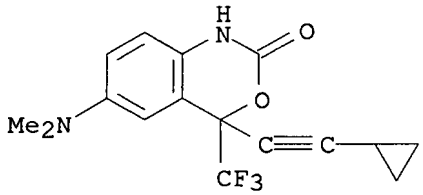
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-methoxy-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



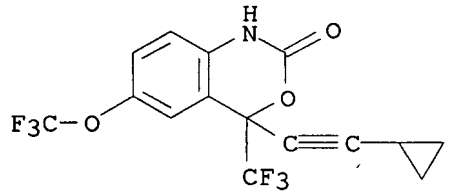
RN 205754-75-2 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-8-fluoro-1,4-dihydro-6-methoxy-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 205754-76-3 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-6-(dimethylamino)-1,4-dihydro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 205754-95-6 CAPLUS
CN 2H-3,1-Benzoxazin-2-one, 4-(cyclopropylethynyl)-1,4-dihydro-6-(trifluoromethoxy)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s efavirenz and (antibod? or hapten or conjugate or carrier)
1512 EFAVIRENZ
500718 ANTIBOD?
10043 HAPTEN
7075 HAPTENS
12806 HAPTEN

```
                (HAPTEN OR HAPTENS)
         70304 CONJUGATE
         63307 CONJUGATES
        109581 CONJUGATE
                (CONJUGATE OR CONJUGATES)
        290352 CARRIER
        164428 CARRIERS
        382568 CARRIER
                (CARRIER OR CARRIERS)
L5         112 EFAVIRENZ AND (ANTIBOD? OR HAPTEN OR CONJUGATE OR CARRIER)

=> s l5 and (antibod? or immunogen or hapten)
        500718 ANTIBOD?
          6679 IMMUNOGEN
          3790 IMMUNOGENS
          9369 IMMUNOGEN
                (IMMUNOGEN OR IMMUNOGENS)
         10043 HAPTEN
          7075 HAPTENS
         12806 HAPTEN
                (HAPTEN OR HAPTENS)
L6          68 L5 AND (ANTIBOD? OR IMMUNOGEN OR HAPTEN)

=> s l6 and immunogen
          6679 IMMUNOGEN
          3790 IMMUNOGENS
          9369 IMMUNOGEN
                (IMMUNOGEN OR IMMUNOGENS)
L7           3 L6 AND IMMUNOGEN

=> s l7 not l4
L8           3 L7 NOT L4

=> d l8 ibib abs hitstr tot

L8   ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:        2007:382300  CAPLUS
DOCUMENT NUMBER:         147:45061
TITLE:                   Development of a competitive immunoassay for
                         efavirenz: Hapten design and
                         validation studies
AUTHOR(S):               Roucairol, Camille; Azoulay, Stephane; Nevers,
                         Marie-Claire; Creminon, Christophe; Grassi, Jacques;
                         Burger, Alain; Duval, Daniele
CORPORATE SOURCE:        Laboratoire de Chimie des Molecules Bioactives et des
                         Aromes, UMR 6001, CNRS-Institut de Chimie de Nice,
                         Universite de Nice-Sophia Antipolis, Nice, Parc
                         Valrose, 06108, Fr.
SOURCE:                  Analytica Chimica Acta (2007), 589(1), 142-149
                         CODEN: ACACAM; ISSN: 0003-2670
PUBLISHER:               Elsevier B.V.
DOCUMENT TYPE:           Journal
LANGUAGE:                English
AB   The reverse transcriptase inhibitor efavirenz (EFV) is widely
     used in human immunodeficiency virus (HIV) therapy.  Knowledge of the
     plasma and intracellular concns. of the drug is of prime importance to get
     further insight into EFV action in vivo and would be useful for
     therapeutic drug monitoring (TDM).  The aim of this study was to develop a
     sensitive and specific competitive enzyme immunoassay (EIA) for EFV in
     biol. fluids.  Two haptens that differed by the position of the
     linker were synthesized using two different ways and coupled to BSA.
     Anti-EFV polyclonal antibodies (pAb) were raised in rabbits
     using the corresponding immunogens.  By comparing results
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obtained with EIA study with those observed with high-performance liquid chromatog. (HPLC) the authors have shown that the position of the linker appears to be crucial for the specificity of the pAb. EIA was then developed in microtitration plates using the most specific pAb. The assay was performed on a min. of 30 μL of plasma. It showed good precision and efficiency as well as good cross-validation with HPLC. The lowest limit of quantification (LLOQ) was 150 pg mL-1, i.e., a value at least 10 times lower than those currently achieved using previously described techniques. This EIA should be useful in the clin. laboratory for monitoring patients during antiretroviral therapy especially young children as well as for measuring EFV in intracellular studies requiring lower amts. of biol. material.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2007:147974 CAPLUS

DOCUMENT NUMBER: 146:265694

TITLE: Quantitative immunoassay to measure plasma and intracellular atazanavir levels: analysis of drug accumulation in cultured T cells

AUTHOR(S): Roucairol, Camille; Azoulay, Stephane; Nevers, Marie-Claire; Creminon, Christophe; Lavrut, Thibault; Garraffo, Rodolphe; Grassi, Jacques; Burger, Alain; Duval, Daniele

CORPORATE SOURCE: Laboratoire de Chimie des Molecules Bioactives et Aromes, UMR 6001, CNRS-Universite de Nice-Sophia Antipolis, Nice, Fr.

SOURCE: Antimicrobial Agents and Chemotherapy (2007), 51(2), 405-411
CODEN: AMACCQ; ISSN: 0066-4804

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We have developed an enzyme immunoassay to measure atazanavir (ATV) levels in plasma and cells. Anti-ATV polyclonal antibodies were raised in rabbits by using a synthetic ATV derivative coupled to bovine serum albumin as the immunogen, and the enzyme tracer was prepared by chemical coupling the ATV derivative with acetylcholinesterase. These reagents were used to develop a sensitive competitive enzyme immunoassay performed in microtitration plates, and the lowest limit of quantification was 150 pg/mL, which is about 10 times more sensitive than previously published techniques. The plasma assay was performed, after a simple methanol extraction, with a min. of 30 μl of plasma. This assay showed good precision and efficiency, since the rates of recovery from human plasma and cell exts. spiked with ATV ranged form 93 to 113%, with coeffs. of variation of less than 10%. ATV concns. were measured in peripheral blood mononuclear cells incubated with various ATV concns. and in CEM cells in the absence or presence of antiretroviral drugs and drug transporter inhibitors. The results indicated a dose-dependent uptake (intracellular concentration/extracellular concentration ratio range, 0.04 to 19). A significant increase in the accumulation of ATV was noticed in the presence of P-glycoprotein and MRP1 inhibitors (dipyridamole, inter alia). Interestingly, efavirenz significantly increased the baseline accumulation of ATV, whereas nevirapine induced a marked reduction This new enzyme immunoassay for measuring plasma and intracellular ATV levels was fully validated and provides an inexpensive and useful tool for routine therapeutic drug monitoring. Moreover, in vitro results suggested the implication of drug transporters and interactions with other antiviral drugs that should be further explored in human immunodeficiency virus-infected patients.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:658930 CAPLUS
TITLE: Reagents for efavirenz immunoassay
AUTHOR(S): Ghoshal, Mitali; Sigler, Gerald; Root, Richard; Ouyang, Anlong; Arabshahi, Lili; Schamerloh, Andrew; Goodman, Joni; Hippensteel, Elizabeth; Tsai, Jane; Passarelli, Joseph
CORPORATE SOURCE: Roche Diagnostics Corporation, Indianapolis, IN, 46250, USA
SOURCE: Abstracts of Papers, 228th ACS National Meeting, Philadelphia, PA, United States, August 22-26, 2004 (2004), ORGN-668. American Chemical Society: Washington, D. C.
CODEN: 69FTZ8
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB Efavirenz (SUSTIVA) plays an important role in combination therapy for the treatment of AIDS. When used with other anti-HIV medicines, efavirenz has been shown to reduce viral load and increase the number of CD4 cell counts in the blood. Although efavirenz, together with other antivirals form an effective combination therapy, clin. research has demonstrated that the virus develops resistance to the drug. A few literature refs. are known for measuring efavirenz plasma concentration by high performance liquid chromatog. methods. It has been reported that treatment failure and CNS side effects were associated with low and high efavirenz plasma level resp. Inter-individual variability in efavirenz levels supports therapeutic drug monitoring (TDM). Our goal is the development of a TDM test for efavirenz based on immunoassay. In this report we describe the synthesis of Efavirenz immunogens (1 & 2), that have been used to produce monoclonal antibodies to efavirenz. These antibodies will be used to develop immunoassays for efavirenz.

=> s l6 and hapten
10043 HAPTEN
7075 HAPTENS
12806 HAPTEN
(HAPTEN OR HAPTENS)
L9 3 L6 AND HAPTEN

=> s l9 not l8
L10 2 L9 NOT L8

=> d l10 ibib abs hitstr tot

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:612004 CAPLUS
DOCUMENT NUMBER: 143:114059
TITLE: Antibodies specific to metabolically sensitive moieties of anti-HIV drugs for immunoassays and haptens comprising the metabolically sensitive moieties
INVENTOR(S): Valdez, Johnny
PATENT ASSIGNEE(S): Ark Diagnostics, USA
SOURCE: PCT Int. Appl., 135 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005062979	A2	20050714	WO 2004-US43576	20041220
WO 2005062979	A3	20060727		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004308507	A1	20050714	AU 2004-308507	20041220
CA 2550316	A1	20050714	CA 2004-2550316	20041220
US 2005244816	A1	20051103	US 2004-19419	20041220
EP 1700122	A2	20060913	EP 2004-815608	20041220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				

PRIORITY APPLN. INFO.:	US 2003-531552P	P	20031219
	WO 2004-US43576	W	20041220

AB This invention provides compds., methods, immunoassays, and kits relating to active, metabolically sensitive ('met-sensitive') moieties of anti-HIV therapeutics, such as HIV protease inhibitors (PI) and HIV non-nucleoside reverse transcriptase inhibitors (NNRTI). Haptens of these anti-HIV therapeutics were prepared for raising monoclonal and polyclonal antibodies for immunoassay.

L10 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	2003:719710 CAPLUS
DOCUMENT NUMBER:	139:244685
TITLE:	Nonpeptide immunologic tracer precursors comprising a tyrosyl-(X)n-lysine or lysyl-(X)n-tyrosine motif, method for preparing them, and uses thereof in immunoassays
INVENTOR(S):	Cupo, Anny; Le Saint, Cecile; Vincent, Jean-Pierre
PATENT ASSIGNEE(S):	Centre National de la Recherche Scientifique -CNRS-, Fr.
SOURCE:	PCT Int. Appl., 37 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	French
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003075010	A2	20030912	WO 2003-FR707	20030305
WO 2003075010	A3	20040506		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,				

BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

FR 2836996	A1	20030912	FR 2002-2783		20020305
AU 2003227812	A1	20030916	AU 2003-227812		20030305
PRIORITY APPLN. INFO.:			FR 2002-2783	A	20020305
			WO 2003-FR707	W	20030305

OTHER SOURCE(S): MARPAT 139:244685

AB The invention discloses an immunol. tracer which comprises a nonpeptide hapten coupled with a Tyr-(X)n-Lys or Lys-(X)n-Tyr motif [X = single bond, amino acid (except for lysine, glutamine, asparagine, Tyrosine), succinyl, citrate, hydroxymethyl group,CH2, O, S, CH2O, CHNH; n = 1-20, preferably 1-10, more preferably 1-2]. The invention also discloses methods for preparing the precursors, as well as their use for preparing immunol. markers useful in competitive immunol. assays.

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=> s l6 and antibod?
        500718 ANTIBOD?
L11          68 L6 AND ANTIBOD?

=> s l11 and immunoassay
          80362 IMMUNOASSAY
          12909 IMMUNOASSAYS
          84245 IMMUNOASSAY
                (IMMUNOASSAY OR IMMUNOASSAYS)
L12          15 L11 AND IMMUNOASSAY

=> s l12 not l10
L13          13 L12 NOT L10

=> s l13 not l9
L14          12 L13 NOT L9

=> s l14 not l8
L15          10 L14 NOT L8

=> d 10 ibib abs hitstr tot

L15  ANSWER 10 OF 10  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2004:452961  CAPLUS
DOCUMENT NUMBER:          141:21840
TITLE:                    Human protein FLJ21908/SHIVA (soluble HIV apoptotic)
                          secreted by HIV-1-infected monocytes, and methods for
                          diagnosing and treating AIDS dementia
INVENTOR(S):              Sperber, Kirk; Gelman, Irwin H.
PATENT ASSIGNEE(S):       USA
SOURCE:                   PCT Int. Appl., 164 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
     WO 2004045519         A2    20040603    WO 2003-US36382          20031113
     WO 2004045519         A3    20050818
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO,
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
             TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
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BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003290876	A1	20040615	AU 2003-290876	20031113
US 2004197770	A1	20041007	US 2003-712671	20031113
EP 1572104	A2	20050914	EP 2003-783461	20031113
EP 1572104	A3	20051005		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.:	US 2002-426103P	P	20021114
	WO 2003-US36382	W	20031113

AB The present invention generally relates to the treatment or inhibition of diseases associated with HIV-1 infection. In particular, the present invention provides methods and compns. for decreasing, inhibiting, or otherwise abrogating neuronal cell apoptosis that leads to HIV-1 associated dementia (HAD). The inventors described a soluble 6000-Da peptide secreted by an HIV-1-infected human macrophages, which induces apoptosis in the neuronal cells, as well as T cells and B cell. The inventors identified this factor as the cDNA clone FL14676485 encoding the human protein, FLJ21908 [now referred to as SHIVA (soluble HIV apoptotic)]. The FLJ21908/SHIVA protein induces apoptosis through activation of caspase-9 and caspase-3. The SHIVA protein can be detected in brain and lymph tissue from HIV-1-infected patients who have AIDS dementia, but not in the neuronal tissue of patients with non-HIV associated dementia. The compns. of the present invention may be used systemically for the treatment of HIV to abrogate neuronal, T and B-cell apoptosis. The compns. of the present invention also may be used to ameliorate inflammatory disorders by inducing cell death in such disorders.

L15 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	2007:521740 CAPLUS
DOCUMENT NUMBER:	147:1978
TITLE:	Method for screening anti-AIDS natural products through identifying HIV-1 reverse transcriptase inhibitor
INVENTOR(S):	Zhang, Wei; Yuan, Jingli; Hu, Zheng; Jin, Yan; Wang, Guilan; Yu, Xingju; Jin, Meifang
PATENT ASSIGNEE(S):	Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Peop. Rep. China
SOURCE:	Faming Zhuanli Shenqing Gongkai Shuomingshu, 10pp. CODEN: CNXXEV
DOCUMENT TYPE:	Patent
LANGUAGE:	Chinese
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1959413	A	20070509	CN 2005-10047612	20051102
PRIORITY APPLN. INFO.:			CN 2005-10047612	20051102

AB Provided is a method for screening anti-AIDS natural products through identifying HIV-1 reverse transcriptase inhibitor. The method comprises the steps of: (1) adding natural products into the reverse transcription reaction system, (2) performing RT-PCR for synthesizing DNA with single-base-composed RNA as template and HIV-1 reverse transcriptase as catalyst, and randomly incorporating biotin-dUTP and digoxigenin-dUTP into DNA to form digoxigenin/biotin-labeled DNA, (3) capturing by specific combination of digoxigenin-labeled DNA and antibody against digoxigenin, and (4) detecting by specific combination of biotin-labeled DNA and fluorescence-labeled streptavidin. The reverse transcriptase reaction system comprises HIV-1 reverse transcriptase, single base-composed RNA, primers, biotin-dUTP, digoxigenin-dUTP, and dTTP. The activity of HIV-1 reverse transcriptase is determined by incorporated

biotin-dUTP in one time unit (the higher the activity, the more incorporated biotin-dUTP in one time unit). This method has the advantages of high efficiency, high sensitivity, simple process, and high antiinterference capability.

L15 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1259342 CAPLUS
DOCUMENT NUMBER: 144:17166
TITLE: Inhibition of HIV-1 replication by disruption of the processing of the viral capsid-spacer peptide 1 protein
INVENTOR(S): Salzwedel, Karl; Li, Feng; Wild, Carl T.; Allaway, Graham P.; Freed, Eric O.
PATENT ASSIGNEE(S): V.I. Technologies, Inc., USA; The Goverment of the United States of America as Represented by the Secretary, Department of Health and Human Services
SOURCE: PCT Int. Appl., 363 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005113059	A2	20051201	WO 2005-US18331	20050524
WO 2005113059	A3	20070215		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005015039	A1	20050120	US 2004-851637	20040524
AU 2005245506	A1	20051201	AU 2005-245506	20050524
CA 2568248	A1	20051201	CA 2005-2568248	20050524
EP 1758640	A2	20070307	EP 2005-779995	20050524
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
CN 101022834	A	20070822	CN 2005-80024103	20050524
NO 2006005982	A	20070201	NO 2006-5982	20061222
IN 2006KN03917	A	20070622	IN 2006-KN3917	20061226

PRIORITY APPLN. INFO.:		
US 2004-851637	A	20040524
US 2005-653961P	P	20050217
US 2003-443180P	P	20030129
US 2003-496660P	P	20030821
US 2004-766528	A2	20040129
WO 2005-US18331	W	20050524

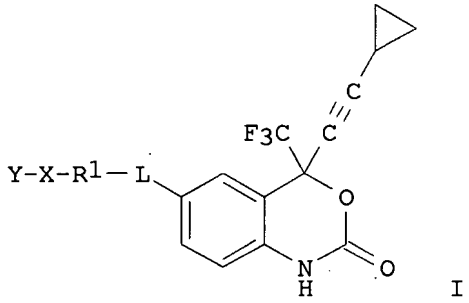
AB Inhibition of HIV-1 replication by disrupting the processing of the viral Gag capsid (CA) protein (p24) from the CA-spacer peptide 1 (SP1) protein precursor (p25) is disclosed. Amino acid sequences containing a mutation in the Gag p25 protein, with the mutation resulting in a decrease in the inhibition of processing of p25 to p24 by dimethylsuccinyl betulinic acid or dimethylsuccinyl betulin, polynucleotides encoding such mutated sequences, and antibodies that selectively bind such mutated sequences are also included. Methods of inhibiting, inhibitory compds.,

and methods of discovering inhibitory compds. that target proteolytic processing of the HIV Gag protein are included. In one embodiment, such compds. inhibit the interaction of the HIV protease enzyme with Gag by binding to Gag rather than to the protease enzyme. In another embodiment, viruses or recombinant proteins that contain mutations in the region of the Gag proteolytic cleavage site can be used in screening assays to identify compds. that target proteolytic processing.

L15 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:527459 CAPLUS
DOCUMENT NUMBER: 143:43890
TITLE: Preparation of 4-cyclopropylethynyl-6-hydroxy-4-trifluoromethyl-1,4-dihydrobenzo[d][1,3]oxazin-2-one derivatives as reagents for detecting efavirenz
INVENTOR(S): Ghoshal, Mitali; Sigler, Gerald; Ouyang, Anlong; Root, Richard
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 19 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005131216	A1	20050616	US 2003-732767	20031210
CA 2489266	A1	20050610	CA 2004-2489266	20041206
EP 1542012	A1	20050615	EP 2004-28897	20041207
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
JP 2005225864	A	20050825	JP 2004-358924	20041210
PRIORITY APPLN. INFO.:			US 2003-732767 A	20031210
OTHER SOURCE(S):	CASREACT 143:43890; MARPAT 143:43890			

GI



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AB The invention provides derivs. of efavirenz (I) [wherein L = NH, O; R1 = (un)saturated, (un)substituted, straight or branched chain of 0-10 carbon or hetero atoms; X = a linker group consisting of 0-2 substituted or unsubstituted aromatic rings or aliphatic linking groups containing 0-10 carbon or hetero atoms; Y = an activated ester, maleimido group, thiol, or NH-Z (where Z = a carrier or a label)] and methods of making efavirenz derivs. The derivs. I include immunogenic compds. for

producing antibodies to efavirenz and labeled efavirenz tracers. These compds. are useful in immunoassay methods for determining efavirenz. Thus, [2-(3-cyclopropyl-1-hydroxy-1-trifluoromethylprop-2-ynyl)-4-(2-methoxyethoxymethoxy)phenyl]carbamic acid tert-Bu ester was cyclized in toluene by treatment with BuLi/hexane at 0-4° for 10 min and at reflux for 1 h to give 4-cyclopropylethynyl-6-(2-methoxyethoxymethoxy)-4-trifluoromethyl-1,4-dihydrobenzo[d][1,3]oxazin-2-one which was deprotected by treatment with CF3CO2H, etherified with Et 4-bromobutyrate in the presence of 18-crown-6 and K2CO3 in acetone at 56° for 3 h, hydrolyzed with LiOH in 50% aqueous MeOH, and acidified with 1 N aqueous HCl to give 4-[(4-cyclopropylethynyl-2-oxo-4-trifluoromethyl-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl)oxy]butyric acid (II). II was esterified with O-(N-succinimidyl)-N,N,N',N'-tetramethyluronium tetrafluoroborate in the presence of diisopropylethylamine in THF to give 4-[[4-(cyclopropylethynyl)-2-oxo-4-trifluoromethyl-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl]oxy]butyric acid 2,5-dioxopyrrolidin-1-yl ester (III). A conjugate prepared from III and keyhole limpet hemocyanin was used to prepare a monoclonal antibody EFA 97.1 specific to efavirenz. The monoclonal antibody EFA 97.1 thus prepared exhibited 100% cross-activity to chiral efavirenz but 0% activity to 3'-azido-3'-deoxythymidine, 2',3'-didehydro-3'-deoxythymidine, nevirapine, delaviridine, nelfinavir, saquinavir, indinavir, ritonavir, amprenavir, lopinavir, and atazanavir which are often coadministered with efavirenz. A serum sample of .apprx.0.2 μL is sufficient to determine efavirenz concentration at 0.0004 to 0.1 μM in a competitive inhibition immunoassay using monoclonal antibody EFA 97.1.

L15 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:123086 CAPLUS
DOCUMENT NUMBER: 142:217394
TITLE: Combined cancer treatment methods using selected antibodies against aminophospholipids
INVENTOR(S): Thorpe, Philip E.; Huang, Xianming; Ran, Sophia
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 182 pp., Cont.-in-part of U.S. Ser. No. 621,269.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2005031620	A1	20050210	US 2003-642058		20030815
US 2004170620	A1	20040902	US 2003-621269		20030715
PRIORITY APPLN. INFO.:			US 2002-396263P	P	20020715
			US 2003-621269	A2	20030715

AB The invention provides new methods and compns. for safe and effective tumor vascular targeting, anti-angiogenesis and tumor destruction, which methods and compns. are also surprisingly effective in treating viral infections and related diseases. The invention is based, in part, on discoveries concerning the expression and role of anionic phospholipids in tumor vasculature and the involvement of aminophospholipids and anionic phospholipids in viral entry, replication and spread. The present invention further provides particularly advantageous antibodies and immunoconjugates that bind to aminophospholipids and anionic phospholipids, and a new class of peptide-based derivs., such as duramycin-based compns., that bind to phosphatidylethanolamine.

L15 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:60015 CAPLUS
DOCUMENT NUMBER: 142:148757
TITLE: Inhibition of HIV-1 replication by disruption of the processing of the viral capsid-spacer peptide 1 protein
INVENTOR(S): Salzwedel, Karl; Li, Feng; Wild, Carl T.; Allaway, Graham P.; Freed, Eric O.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 119 pp., Cont.-in-part of U.S. Ser. No. 766,528.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005015039	A1	20050120	US 2004-851637	20040524
US 2004265320	A1	20041230	US 2004-766528	20040129
AU 2005245506	A1	20051201	AU 2005-245506	20050524
CA 2568248	A1	20051201	CA 2005-2568248	20050524
WO 2005113059	A2	20051201	WO 2005-US18331	20050524
WO 2005113059	A3	20070215		
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1758640	A2	20070307	EP 2005-779995	20050524
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CN 101022834	A	20070822	CN 2005-80024103	20050524
NO 2006005982	A	20070201	NO 2006-5982	20061222
IN 2006KN03917	A	20070622	IN 2006-KN3917	20061226

PRIORITY APPLN. INFO.:

US 2003-443180P	P	20030129
US 2003-496660P	P	20030821
US 2004-766528	A2	20040129
US 2004-851637	A	20040524
US 2005-653961P	P	20050217
WO 2005-US18331	W	20050524

AB Inhibition of HIV-1 replication by disrupting the processing of the viral Gag capsid (CA) protein (p24) from the CA-spacer peptide 1 (SP1) protein precursor (p25) is disclosed. Amino acid sequences containing a mutation in the Gag p25 protein, with the mutation resulting in a decrease in the inhibition of processing of p25 to p24 by dimethylsuccinyl betulinic acid or dimethylsuccinyl betulin, polynucleotides encoding such mutated sequences and antibodies that selectively bind such mutated sequences are also included. Methods of inhibiting, inhibitory compds. and methods of discovering inhibitory compds. that target proteolytic processing of the HIV Gag protein are included. In one embodiment, such compds. inhibit the interaction of the HIV protease enzyme with Gag by binding to Gag rather than to the protease enzyme. In another embodiment, viruses or recombinant proteins that contain mutations in the region of the Gag proteolytic cleavage site can be used in screening assays to

identify compds. that target proteolytic processing.

L15 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:934146 CAPLUS
DOCUMENT NUMBER: 141:409777
TITLE: Aminophospholipid-specific antibodies, immunoconjugates and duramycin-based compounds for treating and diagnosing cancer and viral infections
INVENTOR(S): Thorpe, Philip E.; Ran, Sophia
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 181 pp., Cont.-in-part of U.S. Ser. No. 621,269.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2004219155	A1	20041104	US 2003-642099		20030815
US 2004170620	A1	20040902	US 2003-621269		20030715
PRIORITY APPLN. INFO.:			US 2002-396263P	P	20020715
			US 2003-621269	A2	20030715

AB The invention provides new methods and compns. for safe and effective tumor vascular targeting, anti-angiogenesis and tumor destruction, which methods and compns. are also surprisingly effective in treating viral infections and related diseases. The invention is based, in part, on discoveries concerning the expression and role of anionic phospholipids in tumor vasculature and the involvement of aminophospholipids and anionic phospholipids in viral entry, replication and spread. The present invention further provides particularly advantageous antibodies and immunoconjugates that bind to aminophospholipids and anionic phospholipids, and a new class of peptide-based derivs., such as duramycin-based compns., that bind to phosphatidylethanolamine.

L15 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:898581 CAPLUS
DOCUMENT NUMBER: 141:360649
TITLE: Reagents for detecting efavirenz
INVENTOR(S): Sigler, Gerald F.; Ghoshal, Mitali; Arabshahi, Lili
PATENT ASSIGNEE(S): Roche Diagnostics GmbH, Germany; F. Hoffmann-La Roche Ag
SOURCE: Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 1470825	A1	20041027	EP 2004-9268		20040420
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR					
US 2004214251	A1	20041028	US 2003-420196		20030422
JP 2004323522	A	20041118	JP 2004-124770		20040420
CA 2465017	A1	20041022	CA 2004-2465017		20040421
US 2006088933	A1	20060427	US 2005-255536		20051021
PRIORITY APPLN. INFO.:			US 2003-420196	A	20030422

AB The invention provides derivs. of efavirenz and methods of making derivs. of efavirenz. The derivs. include immunogenic compds. for producing antibodies to efavirenz and

labeled efavirenz tracers. These compds. are useful in immunoassay methods for the detection of efavirenz.
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:681185 CAPLUS
DOCUMENT NUMBER: 141:189647
TITLE: Antibodies specific to aminophospholipids, fragments and immunoconjugates for treating and diagnosing cancer and viral infections
INVENTOR(S): Thorpe, Philip E.; Soares, M. Melina; Ran, Sophia
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 181 pp., Cont.-in-part of U.S. Ser. No. 621,269.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2004161429	A1	20040819	US 2003-642124		20030815
US 2004170620	A1	20040902	US 2003-621269		20030715
PRIORITY APPLN. INFO.:			US 2002-396263P	P	20020715
			US 2003-621269	A2	20030715

AB Disclosed are surprising discoveries concerning the role of anionic phospholipids and aminophospholipids in tumor vasculature and in viral entry and spread, and compns. and methods for utilizing these findings in the treatment of cancer and viral infections. Also disclosed are advantageous antibody, immunoconjugate and duramycin-based compns. and combinations that bind and inhibit anionic phospholipids and aminophospholipids, for use in the safe and effective treatment of cancer, viral infections and related diseases.

L15 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:550531 CAPLUS
DOCUMENT NUMBER: 141:105253
TITLE: Antibodies specific to aminophospholipid and conjugates for diagnosis and treatment of cancer and viral infection
INVENTOR(S): Thorpe, Philip E.; Soares, M. Melina; Ran, Sophia
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 178 pp., Cont.-in-part of U.S. Ser. No. 621,269.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2004131621	A1	20040708	US 2003-642060		20030815
US 2004170620	A1	20040902	US 2003-621269		20030715
PRIORITY APPLN. INFO.:			US 2002-396263P	P	20020715
			US 2003-621269	A2	20030715

AB Disclosed are surprising discoveries concerning the role of anionic phospholipids and aminophospholipids in tumor vasculature and in viral entry and spread, and compns. and methods for utilizing these findings in the treatment of cancer and viral infections. Also disclosed are advantageous antibody, immunoconjugate and duramycin-based

compns. and combinations that bind and inhibit anionic phospholipids and aminophospholipids, for use in the safe and effective treatment of cancer, viral infections and related diseases.

L15 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:452961 CAPLUS
DOCUMENT NUMBER: 141:21840
TITLE: Human protein FLJ21908/SHIVA (soluble HIV apoptotic) secreted by HIV-1-infected monocytes, and methods for diagnosing and treating AIDS dementia
INVENTOR(S): Sperber, Kirk; Gelman, Irwin H.
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 164 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004045519	A2	20040603	WO 2003-US36382	20031113
WO 2004045519	A3	20050818		
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AU 2003290876	A1	20040615	AU 2003-290876	20031113
US 2004197770	A1	20041007	US 2003-712671	20031113
EP 1572104	A2	20050914	EP 2003-783461	20031113
EP 1572104	A3	20051005		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.: US 2002-426103P P 20021114
WO 2003-US36382 W 20031113

AB The present invention generally relates to the treatment or inhibition of diseases associated with HIV-1 infection. In particular, the present invention provides methods and compns. for decreasing, inhibiting, or otherwise abrogating neuronal cell apoptosis that leads to HIV-1 associated dementia (HAD). The inventors described a soluble 6000-Da peptide secreted by an HIV-1-infected human macrophages, which induces apoptosis in the neuronal cells, as well as T cells and B cell. The inventors identified this factor as the cDNA clone FL14676485 encoding the human protein, FLJ21908 [now referred to as SHIVA (soluble HIV apoptotic)]. The FLJ21908/SHIVA protein induces apoptosis through activation of caspase-9 and caspase-3. The SHIVA protein can be detected in brain and lymph tissue from HIV-1-infected patients who have AIDS dementia, but not in the neuronal tissue of patients with non-HIV associated dementia. The compns. of the present invention may be used systemically for the treatment of HIV to abrogate neuronal, T and B-cell apoptosis. The compns. of the present invention also may be used to ameliorate inflammatory disorders by inducing cell death in such disorders.

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FULL ESTIMATED COST                                    135.83      308.14

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 NEWS  3  MAY 08  CA/CAplus Indian patent publication number format defined
 NEWS  4  MAY 14  RDISCLOSURE on STN Easy enhanced with new search and display
                  fields
 NEWS  5  MAY 21  BIOSIS reloaded and enhanced with archival data
 NEWS  6  MAY 21  TOXCENTER enhanced with BIOSIS reload
 NEWS  7  MAY 21  CA/CAplus enhanced with additional kind codes for German
                  patents
 NEWS  8  MAY 22  CA/CAplus enhanced with IPC reclassification in Japanese
                  patents
 NEWS  9  JUN 27  CA/CAplus enhanced with pre-1967 CAS Registry Numbers
 NEWS 10  JUN 29  STN Viewer now available
 NEWS 11  JUN 29  STN Express, Version 8.2, now available
 NEWS 12  JUL 02  LEMBASE coverage updated
 NEWS 13  JUL 02  LMEDLINE coverage updated
 NEWS 14  JUL 02  SCISEARCH enhanced with complete author names
 NEWS 15  JUL 02  CHEMCATS accession numbers revised
 NEWS 16  JUL 02  CA/CAplus enhanced with utility model patents from China
 NEWS 17  JUL 16  CAplus enhanced with French and German abstracts
 NEWS 18  JUL 18  CA/CAplus patent coverage enhanced
 NEWS 19  JUL 26  USPATFULL/USPAT2 enhanced with IPC reclassification
 NEWS 20  JUL 30  USGENE now available on STN
 NEWS 21  AUG 06  CAS REGISTRY enhanced with new experimental property tags
 NEWS 22  AUG 06  BEILSTEIN updated with new compounds
 NEWS 23  AUG 06  FSTA enhanced with new thesaurus edition
 NEWS 24  AUG 13  CA/CAplus enhanced with additional kind codes for granted
                  patents
 NEWS 25  AUG 20  CA/CAplus enhanced with CAS indexing in pre-1907 records
 NEWS 26  AUG 27  Full-text patent databases enhanced with predefined
                  patent family display formats from INPADOCDB
 NEWS 27  AUG 27  USPATOLD now available on STN
 NEWS 28  AUG 28  CAS REGISTRY enhanced with additional experimental
                  spectral property data

 NEWS 29  SEP 07  STN AnaVist, Version 2.0, now available with Derwent
                  World Patents Index
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NEWS EXPRESS 05 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 SEPTEMBER 2007.

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DICTIONARY FILE UPDATES: 9 SEP 2007 HIGHEST RN 946489-93-6

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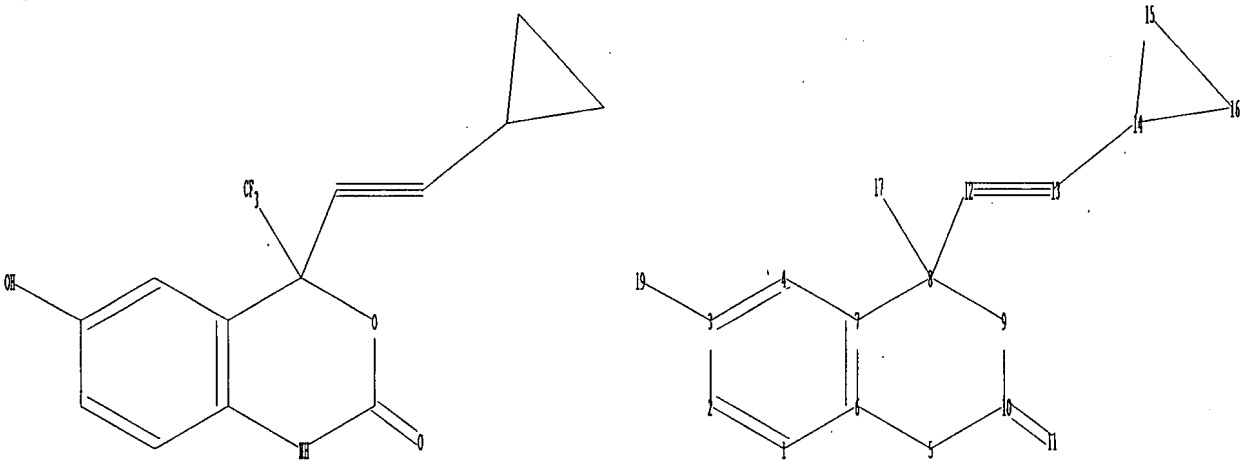

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ring nodes :
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ring bonds :
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exact bonds :
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isolated ring systems :
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Match level :
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11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:CLASS 19:CLASS

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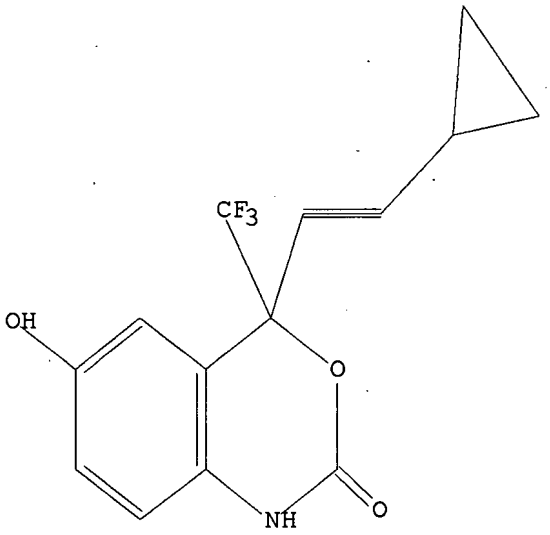

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SEARCH TIME: 00.00.01

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FULL ESTIMATED COST

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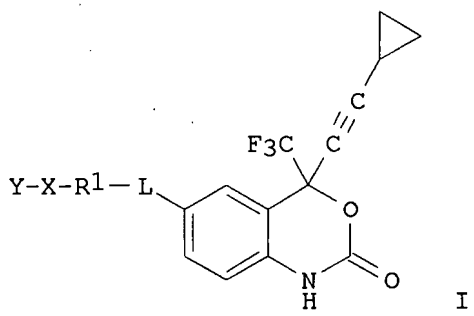
=> s l3
L4 1 L3

=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:527459 CAPLUS
DOCUMENT NUMBER: 143:43890
TITLE: Preparation of 4-cyclopropylethynyl-6-hydroxy-4-trifluoromethyl-1,4-dihydrobenzo[d][1,3]oxazin-2-one derivatives as reagents for detecting efavirenz
INVENTOR(S): Ghoshal, Mitali; Sigler, Gerald; Ouyang, Anlong; Root, Richard
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 19 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005131216	A1	20050616	US 2003-732767	20031210
CA 2489266	A1	20050610	CA 2004-2489266	20041206
EP 1542012	A1	20050615	EP 2004-28897	20041207
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
JP 2005225864	A	20050825	JP 2004-358924	20041210
PRIORITY APPLN. INFO.:			US 2003-732767 A	20031210

OTHER SOURCE(S): CASREACT 143:43890; MARPAT 143:43890
GI



I

AB The invention provides derivs. of efavirenz (I) [wherein L = NH, O; R1 = (un)saturated, (un)substituted, straight or branched chain of 0-10 carbon or hetero atoms; X = a linker group consisting of 0-2 substituted or unsubstituted aromatic rings or aliphatic linking groups containing 0-10 carbon or hetero atoms; Y = an activated ester, maleimido group, thiol, or NH-Z (where Z = a carrier or a label)] and methods of making efavirenz derivs. The derivs. I include immunogenic compds. for producing antibodies to efavirenz and labeled efavirenz tracers. These compds. are useful in immunoassay methods for determining efavirenz. Thus, [2-(3-cyclopropyl-1-hydroxy-1-trifluoromethylprop-2-ynyl)-4-(2-methoxyethoxymethoxy)phenyl]carbamic acid tert-Bu ester was cyclized in toluene by treatment with BuLi/hexane at 0-4° for 10 min and at reflux for 1 h to give 4-cyclopropylethynyl-6-(2-methoxyethoxymethoxy)-4-trifluoromethyl-1,4-dihydrobenzo[d][1,3]oxazin-2-one which was deprotected by treatment with CF3CO2H, etherified with Et 4-bromobutyrate in the presence of 18-crown-6 and K2CO3 in acetone at 56° for 3 h, hydrolyzed with LiOH in 50% aqueous MeOH, and acidified with 1 N aqueous HCl to give 4-[(4-cyclopropylethynyl-2-oxo-4-trifluoromethyl-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl)oxy]butyric acid (II). II was esterified with O-(N-succinimidyl)-N,N,N',N'-tetramethyluronium tetrafluoroborate in the presence of diisopropylethylamine in THF to give 4-[[4-(cyclopropylethynyl)-2-oxo-4-trifluoromethyl-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl]oxy]butyric acid 2,5-dioxopyrrolidin-1-yl ester (III). A conjugate prepared from III and keyhole limpet hemocyanin was used to prepare a monoclonal antibody EFA 97.1 specific to efavirenz. The monoclonal antibody EFA 97.1 thus prepared exhibited 100% cross-activity to chiral efavirenz but 0% activity to 3'-azido-3'-deoxythymidine, 2',3'-didehydro-3'-deoxythymidine, nevirapine, delaviridine, nelfinavir, saquinavir, indinavir, ritonavir, amprenavir, lopinavir, and atazanavir which are often coadministered with efavirenz. A serum sample of .apprx.0.2 μL is sufficient to determine efavirenz concentration at 0.0004 to 0.1 μM in a competitive inhibition immunoassay using monoclonal antibody EFA 97.1.

IT 853655-82-0P, 4-Cyclopropylethynyl-6-hydroxy-4-trifluoromethyl-1,4-dihydrobenzo[d][1,3]oxazin-2-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of efavirenz derivs. as reagents for detecting efavirenz by immunoassay)

RN 853655-82-0 CAPLUS

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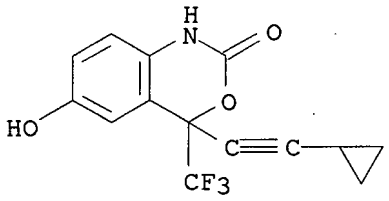

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.74	178.05

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.78	-0.78

STN INTERNATIONAL LOGOFF AT 18:30:48 ON 10 SEP 2007